Appendix E

Management and Characteristics of Beamlines in the Resource

Beamlines at the NSLS are owned, in general, by Participating Research Teams, or PRTs. Each of these supplies the funds to develop, maintain, and operate the beamline, and provides its own management structure. Because the PXRR has integrated the efforts at several beamlines, it will pay to provide details not only about the management and funding source, but also about the capabilities of each beamline in this summary form. Below we tabulate the name of each beamline manager (spokesperson), beamline scientist (local contact) if there is one, principal technician for PX, the PRT members, and then certain details about equipment and operation.

X8-C

1. **Spokesperson:** LeWei Hung, Los Alamos Nat'l Lab
   Tech: Leon Flaks, LANL
   PRT: Integrated Structural Biology Resource (ISBR) of Los Alamos National Laboratory, the DOE Molecular Biology Institute at UCLA , the Biotechnology Research Institute/Institut de recherche en biotechnologie of the National Research Council Canada/Conseil National de Recherche Canada, the Biology Department of Brookhaven National Laboratory, and the Pharmaceuticals Division of Hoffman-La Roche.
2. **Source**: Bending magnet
   Collimating mirror: Bent-plane (cylinder) mirror of fused quartz produces a parallel beam of x-rays from the vertically diverging beam that comes from the synchrotron. This beam nicely matches the narrow rocking curve of the monochromator.
   Existing Monochromator: Two-crystal Si(111).
   Focussing mirror: Bent-cylinder (toroid) focussing mirror, made of fused quartz, coated with Rh.
   Flux: approximately 10^{10} ph/sec through a 0.2mm pinhole.
3. **Equipment**
   Goniometer: Two-axis Crystal-Logic diffractometer (ω and 2θ).
   Detectors: Quantum-4 2×2 array CCD-based detectors
   Cryogenics: An Oxford cryostream specimen cooler
4. **Types of diffraction studies:** Tunable lambda, all types of PX and virus studies.
5. **Other scientific uses:** X8-C operates in both focused and unfocused mode. The latter mode is currently available for general user time, which consitutes 25% of the total operational time. The beamline can be configured to produce a polychromatic beam into the hutch, and it is a large hutch. At the moment this beamline is devoted to monochromatic PX studies, others may be envisioned in coming years.
6. **Software and Computers:** {We intend to make the presentation of the software to the users look as much like beamline X12-C as possible, whatever the underlying codes. This will include integrated control of the κ-axis goniometer, the detector, and the beamline mechanisms. X8-C has now an R4000 and R5000 series SGI computer.} Although X8-C has access to the computing farm, it is rarely used.
7. **Users**
   a. The beamtime will be allocated in the standard PRT mode -- 75% for the PRT and 25% for General Users.

b. Some fraction of this service, perhaps representing 2-5% of total beam time) will be industrial scientists, and a fraction of this (2% of total beam time) will be proprietary research.

X12-B

1. **Spokesperson:** Deiter Schneider, BNL Biology
   Tech: Tom Langdon, BNL Biology
   PRT: Brookhaven Biology Department, funded by the Office of Biological and Environmental Research of the U.S. Dept. of Energy and the NIH National Center for Research Resources
2. **Source**: bending magnet.
   Primary mirror: Single-crystal Si, Rh coated. The mirror is {10cm x 60cm}, and cut to a radius of 3km to produce a collimated beam for both beamlines X12-B and X12-C.
   Monochromator: Small-gap channel-cut Si (111) crystal of the Siddons design, with hybrid analogue-digital feedback loops to maintain tune. Range: 7.5 - 13.1 KeV, bandpass depends on the tune of the collimating mirror. Will range from 2-10 eV.
   Focusing mirror: Dynamically-bent ULE-glass cylinder, Rh coated. Refocuses monochromatic beam to a point ~ 25 meters from tangent point. Spot size 0.3 x 0.3 FWHM (1:1 magnification). Mfg. by Oxford Instruments
   Adaptive collimator: Two-meter evacuated 8" pipe with three sets of **xy** slit screens, mounted from precision gimbals and compound translators. Allows user to select arbitrary collimation geometry.
   Flux: 0.7×10^{10} photon/sec through a 200 μm collimator.
   Pending upgrades: Multilayer monochromator interchangable with Si crystals will be installed during '02-'03 shutdown. 1% bandpass ⇒ 50-fold increase in flux.
3. **Equipment**
   Diffractometer: Locally constructed system -- Track, lift carriage, 3-meter 2θ arm, compound translators, ϕ stage coaxial with 2θ arm - will be upgraded to κ-axis system.
   Detectors: Interchangeable systems -- 1) ADSC Q4 2x2 detector system, 2) MAR 300-mm imaging plate scanner. Two-dimensional multi-wire detector/time-slicing data collection system.
   Cryogenics: Oxford cryosystem, with automatic fill system.
4. **Types of diffraction studies**: Monochromatic (MAD/SAD) crystallography. Long base line (up to 2 meters with He-purged flight paths) 2θ inclinations up to 45 degrees. Very large unit cells (e.g. viruses, large multi component complexes). Measurement of low order, and thermal-diffuse diffraction.
5. **Other scientific uses:** Static and time-resolved small angle diffraction studies on both biological and organic-polymer specimens.
6. **Software and Computers:** The BNL-Bio cbass/grepx system will run the beamline and diffractometer. {The beamline now has two Indy-class Silicon Graphics workstations and one Crimson Elan SGI workstation.} This beamline is a principal user of the computing farm.
7. **Users:**
   a. Biology department PRT (20%)
   b. Collaborators (15%)
   c. Outside users: macromolecular crystallography (65%).

X12-C

1. **Spokesperson:** Robert M. Sweet, BNL Biology
   Local contact: Anand Saxena, BNL Biology
   Tech: Sal Sclafani, BNL Biology
   PRT: Brookhaven Biology Department, funded by the Office of Biological and Environmental Research of the U.S. Dept. of Energy and the NIH National Center for Research Resources
2. **Source**: bending magnet
   Primary mirror: Single-crystal Si, Rh coated. The mirror is {10cm x 60cm}, and cut to a radius of 3km to produce a collimated beam for both beamlines X12-B and X12-C.
   Monochromator: Small-gap channel-cut Si (111) crystal of the Siddons design, with hybrid analogue-digital feedback loops to maintain tune. Range: 7.5 - 13.1 KeV, bandpass depends on the tune of the collimating mirror. Will range from 2-10 eV.
   Focussing mirror: Bent-cylinder (toroid) focussing mirror, made of Glidcop, coated with Pd.
   Possible upgrades: We request funds in this grant cycle to replace the detector/diffractometer system with an ADSC Q210 with Crystal Logic κ-axis diffractometer.
   Flux: approximately 10^{10} ph/sec through a 0.2mm pinhole
3. **Equipment**
   Goniometer: Nonius CAD-4 Style diffractometer, including three-circle crystal orienter, shutter control, collimator, and a meter-long θ-arm to tilt detectors out of the horizonal plane. Rides on a five-axis lift table.
   Detectors: The Brandeis 2k-square CCD-based detector. We hope to purchase a new large-format detector under this grant.
   Cryogenics: New Oxford Instruments Cryo___ cryogenic system.
4. **Types of diffraction studies:** Tunable lambda, all types of PX and virus studies. MAD data collected automatically. Can collect high-resolution data to 0.7Å; low resolution data to 300-Å resolution.
5. **Other scientific uses:** Some (1-5%) small-molecule diffraction studies.
6. **Software and computers:** We have developed our own integration for beamline-control, data-collection, and data-reduction software. All of this has depended on incorporation of well established codes into a seamlessly integrated, easily controlled GUI-based software system. The current system runs on SGI machines in a Unix environment. We don't feel constrained by this, and will likely migrate toward Intel linux. The goal will continue to be to provide reliable software in which our users feel confidence. {The beamline now has two Indy R4000 series and one R5000 series Silicon Graphics workstation. } This beamline is a principal user of the computing farm.
7. **Users**
   a. The PRT includes members of the BNL Biology department. We will be using approximately 20% of the beam time.
   b. Our collaborators will use approximately another 20%.
   c. The remainder (60%) will be service. Some fraction of this, perhaps representing 5-10% of total beam time) will be industrial scientists, and a fraction of this (2-5% of total beam time) will be proprietary research.

X25

1. **Spokesperson:** Lonny Berman, National Synchrotron Light Source
   Local contact for PX: Michael Becker, BNL Biology
   Tech for PX: Shai Vaday, BNL Biology

PRT: The National Synchrotron Light Source, funded by the Office of Basic Energy Sciences of the U.S. Dept. of Energy, and Brookhaven Biology Department, funded by the Office of Biological and Environmental Research of the U.S. Dept. of Energy and the NIH National Center for Research Resources

2. **Source**: X25 source is a 27-pole wiggler that produces an emission spectrum similar to that of the NSLS bending magnets.
   Focussing mirror: Bent-cylinder (toroid) focussing mirror, made of single-crystal silicon, coated with Pt.
   Monochromator: Two-crystal Si(111). First crystal is adaptively bent to accommodate the heat load. The mirror precedes the monochromator; the bandwidth is slightly larger than with the opposite configuration.
   Possible upgrades: A major component of this proposal is to replace the wiggler with a mini-gap undulator, which should produce a beam three to five times as bright as the wiggler in the spectral range useful for PX.
   Flux: Doubly-focussed integrated flux at 300 mA current is $4x10^{12}$ ph/sec at 8 keV using a Si(111) monochromator, and $2x10^{12}$ ph/sec at 12 keV. The fluxes transmitted through a 250-μm square collimator, as normally used for protein crystallography, are about 10 times lower than the integrated fluxes quoted above. The NSLS x-ray ring current is expected to reach its saturation value of 440 mA current in about one year.
3. **Equipment**, all dedicated to this beamline and likely to be still there 3-4 years from now. These include the six-circle diffractometer, and SGI and Pentium computers, as well as an assortment of simple x-ray detectors such as ion chambers, scintillators, and PIN diodes.
   Goniometer: The diffractometer system is an ADSC / Crystal Logic κ-axis diffractometer on a six-motor lift table.
   Detectors: ADSC Q315 CCD-based detector. This and its diffractometer were purchased within the last year from funds contributed by a range of agencies, including DOE/BER, NIH/NCRR, and NIH/NIGMS.
   Cryogenics: The existing specimen cooler is by Oxford Cryosystems.
4. **Types of diffraction studies:** Under this Resource, at least half of the X25 beam time is assigned to macromolecular crystallography. All types of tunable-λ PX and virus studies are performed. If the increased personnel requested in this proposal are granted, the beamline will become 100% devoted to PX.
5. **Other scientific uses:** Roughly half of X25's beam time is assigned to diffraction and scattering studies of condensed matter systems.
6. **Software and computers:** For beamline control, X25 PX users employ the BNL-produced cbass/GRACE system. The beamline-control hardware is being upgraded so that the **cbass**/GrEpx software package like that at beamline X12-C will be the standard. {Two SGI R5000 machines are available now.} This beamline is a principal user of the computing farm.
7. **Users**
   a. The PRT includes the beamline spokesperson and his department in the NSLS. Approximately 15% of the beamtime is used for beamline-development by the PRT.
   b. Approximately 15% of the time is used for collaborative research.
   c The remainder (70%) is assigned as service based on competitive proposals to the NSLS General User Program. Perhaps 5% of X25 beam time is used by industrial scientists.

X26-C

1. **Spokesperson:** Dieter Schneider, BNL Biology
   Local contact: Annie Héroux, BNL Biology
   PRT: BNL Biology Dept., Cold Spring Harbor Laboratory, SUNY Stony Brook, Georgia Research Alliance.
2. **Source**: bending magnet
   Monochromator: Small-gap channel-cut Si (111) crystal of the Siddons design, with hybrid analogue-digital feedback loops to maintain tune. Range: 7.5 - 13.1 KeV, bandpass will depend on slits used: 3-15 eV. This monochromator is easily removed (½ day's work) to provide for focussed polychromatic x-rays for white-beam Laue-diffraction studies.
   Focussing mirror: Bent cylinder of single-crystal silicon, 1.2m long. This mirror can easily be removed (3hr work) to provide a highly collimated beam for three-beam diffraction and crystal characterization.
   Flux: approximately 5×10^{10} ph/sec through a 0.2mm pinhole.
3. **Equipment**
   Goniometers: 1) Nonius CAD-4 Style diffractometer, including three-circle crystal orienter, shutter control, collimator, and a meter-long θ-arm to tilt detectors out of the horizonal plane. This instrument is identical to that installed on X12-C now. This is mounted on a six-motor lift table. 2) Six-circle Huber ψ-axis diffractometer used for the three-beam diffraction project. The two diffractometers are exchangeable in about a day's work.
   Detectors: ADSC Q4 CCD-based detector. KI and YAP detectors for the ψ-axis diffractometer
   Cryogenics: The specimen cooler is by Oxford Cryosystems.
4. **Types of diffraction studies:** Tunable lambda, all types of PX and virus studies. White-beam Laue diffraction studies. Multi-beam diffraction.
5. **Other scientific uses:** Just the wide range described in 4.
6. **Software and computers:** The BNL Biology cbass/grepx system is used; this was the original beamline using this modern, integrated system. {computers??}
7. **Users**
   a. The four members of the PRT each use a 19% share of the beam time.
   b. The remainder (25%) is service. Some fraction of this, perhaps representing 2-5% of total beam time) will be industrial scientists, and a fraction of this (2% of total beam time) will be proprietary research.

X29

1. **Spokesperson:** Mark Chance, AECOM
   Local Contact: Robert Sweet, BNL Biology
   PRT: AECOM, BNL Biology, NSLS
2: **Source:** In-vacuum x-ray undulator (MGU)
   Monochromator: Two-crystal Si(111). First crystal is cooled to cryogenic temperature using a closed-cycle helium refrigerator. Second crystal can be sagittally curved to focus the beam horizontally at 2:1 demagnification in the end station.
   Focusing mirror: Bendable flat substrate which can be bent to an ellipse to focus the beam vertically at 3:1 demagnification. Substrate to have one metal coating stripe and one uncoated stripe.
3. **Equipment**
   Goniometer: Crystal Logic kappa-axis diffractometer on a motorized optical table.
   Detector: ADSC Q315 9-cell CCD detector.

Cryogenics: Oxford Cryosystems cryostream or Oxford Instruments cryojet.

4. **Types of diffraction studies**: Standard PX, MAD, large unit cells.
5. **Other scientific uses:** A percentage of the beam time will be used in white-beam mode for biological footprinting.
6. **Software and computers:** Software will be almost identical to that at X25. This beamline will be brought into operation early in 2004. The precise complement of local computers and storage has not been decided. It will be designed to provide several "seats" for access to the computing farm, and some local computing, disk storage, and backup capability in case of network failure. EPICS / **cbass** / GrEpx for beamline and experiment control with its Motorola/VME CPU.
7. **Users:** The PRT will focus on operating the best possible General User program while meeting the objectives of the PXRR. A likely division of beam time:
   - 60% to be assigned as service, based on proposals submitted to the NSLS General User Program.
   - 10% for structural genomics by the NYSGRC
   - 15% for biological footprinting
   - 7.5% for local and collaborative projects
   - 7.5% for maintenance and R&D